Damping the zero-point energy of a harmonic oscillator

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The thermal and zero-point energy of a damped harmonic oscillator are calculated for a range of damping values from zero to infinity. Both the thermal and zero-point energies decrease with damping. The energy stored in the quantum damped oscillator at fixed temperature increases with damping, an effect that may be experimentally observable. As the results follow from canonical quantization, the uncertainty principle is valid for all damping levels.

PACS numbers: 03.65.-w, 03.65.Yz, 03.70.+k

The one-dimensional damped harmonic oscillator has a central place in physics due to its simplicity and wide range of application. Although the classical treatment of this dynamical system is elementary and its application to classical behaviour is well understood, the opposite is true in quantum physics. The dissipation of energy leads to difficulties in applying the standard quantization rules to the damped oscillator [1–21], and experimental damped quantum oscillators are probing the degree to which quantum mechanics describes the macroscopic world [22–26].

The technical difficulties in the canonical quantization of the damped harmonic oscillator can be overcome by inclusion of reservoir degrees of freedom that take up the dissipated energy. If the reservoir has a finite, or countably infinite, number of degrees of freedom then a delicate limiting procedure must be employed to capture a wide range of damping behaviour [3, 10–20] (this limit is usually dealt with briskly, but the subtleties involved are lucidly demonstrated by Tatarskii [13]). The limiting procedure amounts to a transition from a countably infinite to an uncountably infinite number of dynamical degrees of freedom in the reservoir. In [21] a reservoir with an uncountably infinite number of degrees of freedom [27] was used from the outset, thus removing any need for a limiting operation. The resulting theory has many similarities with macroscopic electromagnetism, which can be viewed as a field theory of damped oscillators. In particular, the dynamics of a general damped harmonic oscillator is governed by an arbitrary susceptibility that obeys Kramers-Kronig relations [21], just as for the dynamics of light in a material medium. Canonical quantization of macroscopic electromagnetism for arbitrary dielectrics [28, 29] and canonical quantization of a general damped harmonic oscillator [21] can both be directly achieved using the powerful reservoir formalism introduced in [27].

In this paper we apply the general results for a quantum damped harmonic oscillator in thermal equilibrium [21] to a simple example and show that the zero-point energy of the oscillator is less than $\hbar\omega_0/2$, where ω_0 is the free oscillation frequency in the absence of damping. The energy removed in cooling the oscillator from temperature $T > 0$ to its quantum ground state increases with damping, which offers one possibility of experimentally demonstrating the effect derived here.

Following [21] we consider a damped harmonic oscillator with unit mass, free oscillation frequency ω_0 and position operator $\hat{q}(t)$. The canonical momentum $\hat{\Pi}_q(t)$ is equal to the velocity and the canonical quantization relation $[\hat{q}(t), \hat{\Pi}_q(t)] = i\hbar$ is satisfied [21]. In thermal equilibrium the expectation values of the squares of the position and momentum operators are [21]

$$\left\langle \hat{q}^2(t) \right\rangle = \frac{\hbar}{\pi} \int_0^\infty d\omega \coth\left(\frac{\hbar\omega}{2k_B T}\right) \mathrm{Im}G(\omega), \tag{1}$$

$$\left\langle \hat{\Pi}_q^2(t) \right\rangle = \frac{\hbar}{\pi} \int_0^\infty d\omega\, \omega^2 \coth\left(\frac{\hbar\omega}{2k_B T}\right) \mathrm{Im}G(\omega) \tag{2}$$

where $G(\omega)$ is a Green function

$$G(\omega) = \frac{-1}{\omega^2 - \omega_0^2\left[1 - \chi(\omega)\right]} \tag{3}$$

determined by an arbitrary susceptibility $\chi(\omega)$ that obeys Kramer-Kronig relations. When the damping is zero the susceptibility $\chi(\omega)$ vanishes and the Green function (3) is that of a free oscillator of frequency ω_0. The energy of the oscillator in thermal equilibrium must be obtained from the total thermal energy of the coupled oscillator/reservoir system. A simple prescription for performing this calculation was used in [21], and amounts to subtracting from the total thermal energy the thermal energy of the reservoir in the absence of any coupling to the oscillator. This gives the result [21]

$$\langle \hat{H} \rangle_q = \frac{\hbar}{2\pi} \int_0^\infty d\omega \coth\left(\frac{\hbar\omega}{2k_B T}\right) \times \mathrm{Im}\left\{ \left[\omega_0^2 \left(\omega \frac{d\chi(\omega)}{d\omega} - \chi(\omega) + 1 \right) + \omega^2 \right] G(\omega) \right\}. \tag{4}$$

A similar procedure in the electromagnetic case gives the Casimir (zero-point plus thermal) stress-energy of the electromagnetic field in a material [28]. In the Appendix we show that the prescription giving (4) is equivalent to the thermal average of the Hamiltonian of mean force [30], consistent with earlier work on the thermodynamics of strongly coupled systems [31]. In light of this, the results in [28] show that the Casimir energy density is the thermal average of the Hamiltonian of mean force for the electromagnetic field in a macroscopic medium.

The susceptibility $\chi(\omega)$ of an experimental damped oscillator must be measured rather than postulated, just as the electromagnetic susceptibility of an individual material sample must be measured (and will vary even for samples of the same material). The position and momentum correlation functions [21] of the damped oscillator in thermal equilibrium provide one method of experimentally extracting $\chi(\omega)$ and ω_0 that appear in (3). It is nevertheless useful to consider simple formulae for the susceptibility of a damped oscillator, as is widely done in the electromagnetic case. In [21] the example of damping proportional to velocity was treated in detail, but this gives some problems with the zero-damping limit at $T > 0$ if the corresponding susceptibility $\chi(\omega)$ is taken to hold strictly at all frequencies up to infinity. The susceptibility ceases to be physically meaningful at very high frequencies and therefore the high-frequency part of $\chi(\omega)$ should have no physical consequences. In addition, the case of damping proportional to velocity would not be expected to be experimentally relevant [21]. We therefore here consider another example, chosen to be simple enough to allow exact analytical solution while being well-behaved in the limit of zero damping of the oscillator.

We consider the susceptibility

$$\chi(\omega) = \frac{2\gamma_2(\gamma_1^2 + \omega_0^2)}{\omega_0^2(\gamma_1 + 2\gamma_2 - i\omega)}, \tag{5}$$

where γ_1 and γ_2 are positive real constants. Being analytic on the upper-half complex-frequency plane, the real and imaginary parts of (5) exhibit Kramer-Kronig relations and we can write

$$\omega_0^2\,\chi(\omega) = \mathrm{P}\int_0^\infty d\xi \frac{\alpha^2(\xi)}{\xi^2 - \omega^2} + \frac{i\pi\alpha^2(\omega)}{2\omega}, \tag{6}$$

where $\alpha(\omega)$ is the function that couples the displacement q of the oscillator to the reservoir [21]. For (5) the coupling function is

$$\alpha(\omega) = \sqrt{\frac{4\gamma_2\omega^2(\gamma_1^2 + \omega_0^2)}{\pi[(\gamma_1 + 2\gamma_2)^2 + \omega^2]}}. \tag{7}$$

The thermal results (1), (2) and (4) were derived in [21] for cases where the total Hamiltonian is diagonalizable, a sufficient condition for which is the inequality

$$\omega_0^2 > \int_0^\infty d\xi \frac{\alpha^2(\xi)}{\xi^2}. \tag{8}$$

For the coupling function (7) the condition (8) yields

$$\omega_0^2 > 2\gamma_1\gamma_2, \tag{9}$$

so we impose this in what follows. When $\gamma_2 \to 0$, γ_1 remaining fixed, the susceptibility (5) vanishes and the case of an undamped oscillator is recovered.

The Green function (3) for the susceptibility (5) has poles

$$\omega = -i\gamma_1, \quad \omega = -i\gamma_2 \pm \omega 1, \tag{10}$$

$$\omega_1 = \sqrt{\omega_0^2 - \gamma_2(2\gamma_1 + \gamma_2)}. \tag{11}$$

The constants γ_1 and γ_2 thus serve as damping constants of the oscillator, while ω_1 is a modified oscillation frequency when it is real. Note that (9) implies that the poles (10) are all in the lower-half complex-frequency plane so the Green function has retarded boundary conditions. The over-damped case with imaginary ω_1 can also occur while satisfying (9).

The thermal expectation values (1), (2) and (4) can all be evaluated analytically for the susceptibility (5). The integrands in each case are even functions of ω for $T > 0$ and so can be rewritten with lower integration limit of $-\infty$; the integrals are then evaluated by closing the integration contour in the upper (or lower) half-plane. The infinite sum over the residues of the poles of the hyperbolic cotangent function can be expressed in terms of harmonic numbers, but the resulting expressions are rather lengthy. In the limit $\gamma_2 \to 0$, the expectation values (1), (2) and (4) reduce to the free-oscillator values $(\hbar/2\omega_0)\coth(\hbar\omega_0/2k_BT)$, $(\hbar\omega_0/2)\coth(\hbar\omega_0/2k_BT)$ and $(\hbar\omega_0/2)\coth(\hbar\omega_0/2k_BT)$, respectively (the momentum-squared expectation value is equal to the thermal energy for a free oscillator with unit mass, but for non-zero γ_2 these two quantities are different). The thermal energy as a function of the damping γ_2 is plotted for temperature $T = \hbar\omega_0/k_B$ in Fig. 2.

The zero-point ($T = 0$) values of (1), (2) and (4) are most easily calculated directly rather than as the $T \to 0$ limits of the thermal results. The zero-point results are

$$\left\langle \hat{q}^2(t) \right\rangle = \frac{\hbar}{\pi\omega_1(\omega_0^2 + \gamma_1^2 - 4\gamma_1\gamma_2)} \left[(\omega_1^2 + \gamma_1^2 - \gamma_2^2)\arctan\left(\frac{\omega_1}{\gamma_2}\right) + \gamma_2\omega_1 \ln\left(\frac{\omega_0^2 - 2\gamma_1\gamma_2}{\gamma_1^2}\right)\right], \tag{12}$$

$$\left\langle \hat{\Pi}_q^2(t) \right\rangle = \frac{\hbar}{\pi\omega_1(\omega_0^2 + \gamma_1^2 - 4\gamma_1\gamma_2)} \left\{ \left[(\omega_1^2 + \gamma_2^2)^2 + \gamma_1^2(\omega_1^2 - \gamma_2^2)\right] \arctan\left(\frac{\omega_1}{\gamma_2}\right) - \gamma_1^2\gamma_2\omega_1 \ln\left(\frac{\omega_0^2 - 2\gamma_1\gamma_2}{\gamma_1^2}\right)\right\}, \tag{13}$$

$$\langle \hat{H} \rangle_q = \frac{\hbar}{2\pi} \left\{ 2\omega_1 \arctan\left(\frac{\omega_1}{\gamma_2}\right) + \gamma_1 \ln\left(1 + 2\frac{\gamma_2}{\gamma_1}\right) + \gamma_2 \ln\left[\frac{(\gamma_1 + 2\gamma_2)^2}{\omega_0^2 - 2\gamma_1\gamma_2}\right]\right\}. \tag{14}$$

We recall that these expressions presuppose the inequality (9) and note that they are real in the over-damped case where ω_1

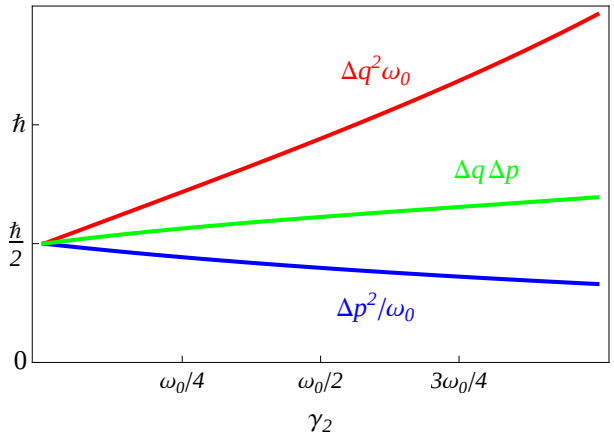

FIG. 1: Plots of the zero-point position uncertainty Δq (square root of (12)) and momentum uncertainty Δp (square root of (13)) versus damping γ_2 with $\omega_0 = 10^{10}\,\mathrm{s}^{-1}$ and $\gamma_1 = \omega_0/4$. The squares of the uncertainties are scaled with an appropriate power of ω_0 to have the same units as the product $\Delta q\,\Delta p$. The uncertainty relation is satisfied for all parameters obeying (9).

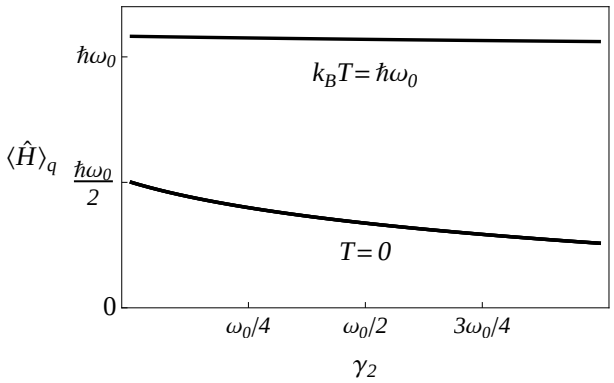

FIG. 2: Plots of the energy of the harmonic oscillator versus damping γ_2, with $\omega_0 = 10^{10}\,\mathrm{s}^{-1}$ and $\gamma_1 = \omega_0/4$, for $T = 0$ and $T = \hbar\omega_0/k_B$. The zero-point energy ($T = 0$) is damped below the free-oscillator value $\hbar\omega_0/2$. The energy for $T > 0$ is also damped below the free-oscillator value, though this damping is not very apparent except for very low T. The energy that can be extracted from the oscillator at $T > 0$ (i.e. the $T > 0$ energy minus the zero-point energy) increases with damping.

is imaginary.

Since all results here are derived from canonical quantization, the position/momentum uncertainty relation holds for the quantum damped oscillator. The squares Δq^2 and Δp^2 of the position and momentum uncertainties are given by (12) and (13), respectively. Figure 1 shows the uncertainties as a function of γ_2 for $\omega_0 = 10^{10}\,\mathrm{s}^{-1}$ and $\gamma_1 = \omega_0/4$. As damping (γ_2) increases the product $\Delta q\,\Delta p$ increases from the minimum allowed value $\hbar/2$. The position uncertainty Δq increases with damping while Δp decreases.

The zero-point energy (14) of the oscillator is plotted in Fig. 2 as a function of γ_2 for $\omega_0 = 10^{10}\,\mathrm{s}^{-1}$ and $\gamma_1 = \omega_0/4$; the energy at temperature $T = \hbar\omega_0/k_B$ is also plotted. As γ_2 increases the zero-point energy is damped below the free-oscillator value $\hbar\omega_0/2$. In our example the oscillation frequency for $\gamma_2 > 0$ is ω_1, given by (11), provided ω_1 is real. But the zero-point energy of the damped oscillator is not $\hbar\omega_1/2$, as is clear from (14). In fact the range of γ_2 in Fig. 2 passes through $\omega_1 = 0$ and into the over-damped case where ω_1 is imaginary. The energy at $T > 0$ is also damped below the free-oscillator value but the difference between the $T > 0$ energy and the zero-point energy increases with damping. This shows that the energy stored in the oscillator at fixed T increases with damping, and this energy must be removed to bring the oscillator to its ground state.

We can also consider the limit of infinite damping, which occurs when $\gamma_2 \to \infty$. The condition (9) then requires $\gamma_1 \to 0$, which we can satisfy by setting $\gamma_1 = \omega_0^2/(4\gamma_2)$ for example. With this value for γ_1, the zero-point energy (14) goes to zero for infinite damping $\gamma_2 \to \infty$, with a leading term of

$$\langle\hat{H}\rangle_q \sim \frac{\hbar\omega_0^2}{4\pi\gamma_2}\left[1 + 2\ln\left(\frac{2^{3/2}\gamma_2}{\omega_0}\right)\right]. \qquad (15)$$

The asymptotic approach of the zero-point energy to zero as $\gamma_2 \to \infty$ is thus very slow. We must note however that the position uncertainty diverges as $\Delta q \sim 2\sqrt{\hbar\gamma_2/\pi}/\omega_0$ in this infinite-damping limit (with $\gamma_1 = \omega_0^2/(4\gamma_2)$). A large displacement of the oscillator can be expected to lead to nonlinear behaviour, so our assumption of a linear oscillator is not realistic for extremely large damping with susceptibility (5).

As noted at the outset, the susceptibility is a quantity that must be measured, and in addition the "free-oscillation" frequency ω_0 is a parameter that must also be fitted to experimental data [21]. The theoretical ideal is a oscillator whose damping can be tuned from zero to a desired level, but this is a heavy demand in practice. A more realistic scenario is a set of macroscopic oscillators prepared with slightly different material geometries so that the damping varies slowly across the set. In the absence of data for the susceptibilities of such a set of oscillators, the results for the simple susceptibility (5) give some qualitative indications. The results in Fig. 2 suggest that if all oscillators in the set are brought to a fixed temperature, then the energy removed from the oscillators in reaching their ground states will increase with damping, where the damping level is determined from the measured susceptibilities.

We are indebted to J. Anders for informing us of the Hamiltonian of mean force. We also thank N. Kiesel and M. Aspelmeyer for interesting discussions.

Appendix

Consider a system composed of two interacting parts; the system of interest (S), and a reservoir (R). The total Hamiltonian of this system is of the form, $\hat{H} = \hat{H}_S + \hat{H}_I + \hat{H}_R$, where $\hat{H}_I$ characterises the coupling (of arbitrary strength) between

S and the reservoir. We ask the question, *what is the energy of S in thermal equilibrium*?

A choice of Hamiltonian, $\hat{H}^\star$ that gives the correct equilibrium properties for S without reference to R is the Hamiltonian of mean force [30]

$$\hat{H}^\star = -\beta^{-1}\log\left(Z_R^{-1}\mathrm{Tr}_R\left[e^{-\beta\hat{H}}\right]\right) \tag{A.16}$$

where $\beta = 1/kT$, and $Z_R = \mathrm{Tr}_R[\exp(-\beta\hat{H}_R)]$. The partition function $Z^\star$ associated with $\hat{H}^\star$ is then

$$Z^\star = \mathrm{Tr}_S\left[e^{-\beta\hat{H}^\star}\right] = \frac{Z}{Z_R}, \tag{A.17}$$

where $Z = \mathrm{Tr}[\exp(-\beta\hat{H})]$ is the total partition function. It is evident that equilibrium averages of quantities pertaining to S alone, computed using $\hat{H}^\star$ will be identical to those calculated from the full Hamiltonian $\hat{H}$. The factor of Z_R^{-1} within the logarithm plays no role in such a calculation, but is determined by the requirements that (a) when $\hat{H}_I \to 0$ then $\hat{H}^\star \to \hat{H}_S$; and (b) the free energy $F^\star$ associated with S is [31]

$$F^\star = -\beta^{-1}\log(Z^\star) = F - F_R, \tag{A.18}$$

which is the amount of energy available to do work in a reversible, isothermal change of state of S, including that obtained through decoupling S and R [31]. In the case considered in the main text, where the q-oscillator plays the role of S, (A.18) will give the correct generalized force (and therefore work done during any isothermal change of state) when $F^\star$ is differentiated with respect to the "free-oscillation" frequency ω_0, or the quantities $\gamma_{1,2}$ within the coupling of the oscillator to the reservoir. Furthermore, when $\gamma_{1,2} \to 0$ then $F^\star \to F_S$.

Given the above properties, (A.16) is interpreted as the effective Hamiltonian of S in thermal equilibrium. In answer to our initial question, the equilibrium average of the associated energy is, using (A.17),

$$\langle\hat{H}^\star\rangle = -\frac{\partial\log(Z/Z_R)}{\partial\beta} = \langle\hat{H}\rangle - \langle\hat{H}_R\rangle, \tag{A.19}$$

where $\langle\hat{H}_R\rangle = -\partial\log(Z_R)/\partial\beta$ is the equilibrium average of the energy of R in the absence of any coupling to S. This is the prescription that was previously used to calculate the Casimir energy density [28] and the thermal energy of a damped harmonic oscillator [21], the latter of which is given by (4).

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